

## **Diels - Alder reaction: Effect of internal and external factors on the reactivity of diene - dienophile systems**

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### **Abstract**

The key factors influencing the Diels - Alder reaction rate at ambient and elevated pressures were elucidated using data on the reactivity of various diene - dienophile systems in usual and Lewis acid-catalyzed Diels-Alder reactions, the reaction enthalpy, complex formation, dissolution, and solvation, and the donor-acceptor properties of the reactants. It was found that taking account of both the orbital interaction energy and the balance of bond rupture and formation energies allows correct prediction of the reaction rate in the absence or in the presence of Lewis acids.

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### **Keywords**

Activation volumes, Catalysis, Diels - Alder reaction, Kinetics, Molecular complexes, Reaction enthalpy, Reaction volumes